# *FOURIER TRANSFORM MICROWAVE LABORATORY DETECTION OF $HSiNH_2$*

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# *Why $HSiNH_2$ ??*

- ✓ Laboratory work driven by astronomical interest
- ✓ So far more than 10 Si-bearing molecules observed in the ISM
- ✓ *SiN* radical detected in circumstellar envelope and galactic center

*(Turner, ApJ 1992; Schilke et al. A&A 2003)*

- ✓ mm- and submm- spectrum of *HNSi* detected by Bogey et al. mixing silane and nitrogen (A&A, 1991)
- ✓ Recently in our lab FTMW measurements of 7 isotopic species and more than 30 vibrational-excited states (see *RC09 - S. Thorwirth*)
- ✓ Attempt to detect *HSiN*, 3 eV higher in energy than the ground state

# *Theoretical studies*

✓ Several theoretical works analyzed the [3H, Si, N] system

✓ The *$HSiNH_2$* planar $C_s$ isomer is the ground state with the *$HNSiH_2$* around 20 kcal/mol higher in energy

*(Truong & Gordon, JACS 1986)*

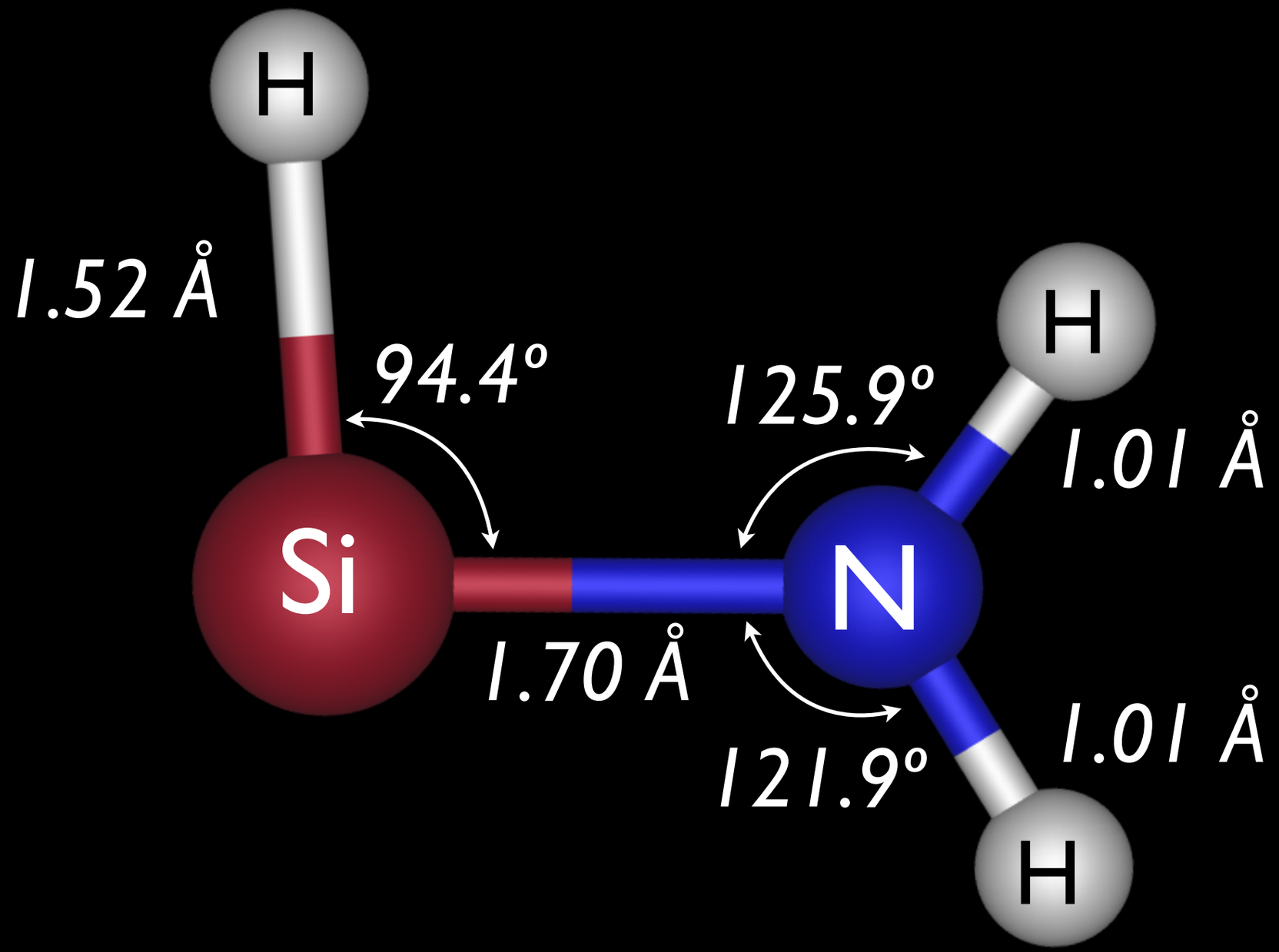
✓ Electronic absorption spectrum observed using matrix isolation IR spectroscopy

*(Maier et al. Chem. Ber. 1989)*

✓ New theoretical structure calculations performed at the CCSD(T)/cc-pwCVQZ level of theory

✓Structure corrected for zero-point vibrational effects at the CCSD(T)/cc-pV(T+d)Z level.

# Calculated Structure

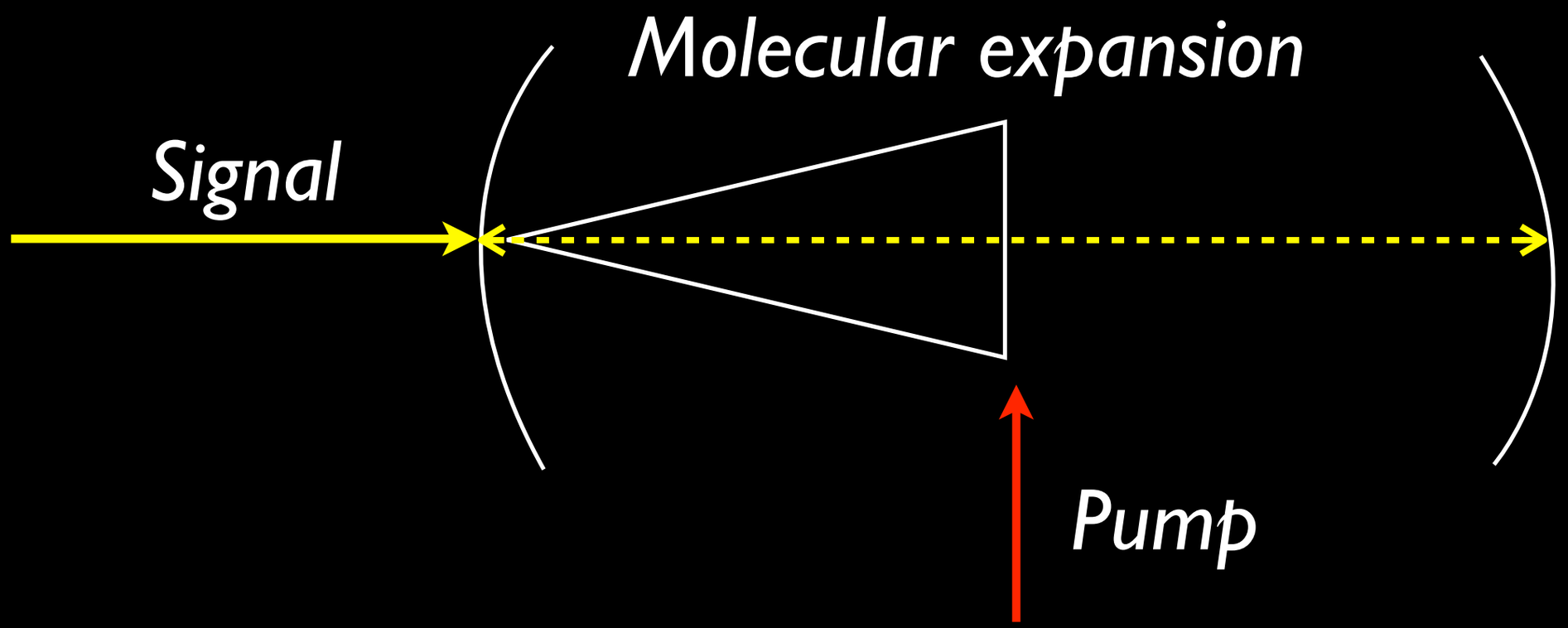


# *Experimental setup - FTMW*

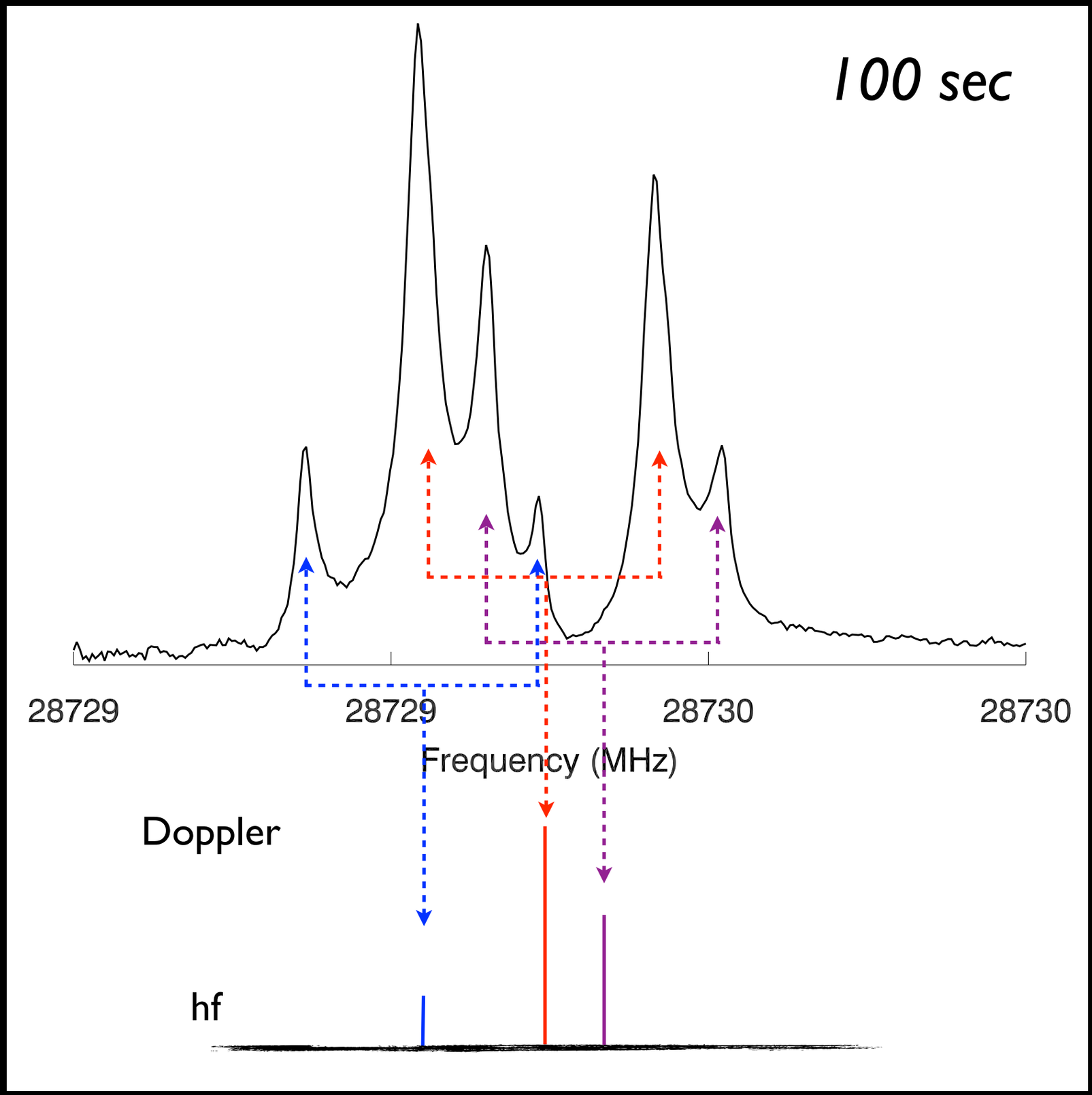
- ✓ Detection of the rotational spectra by FTMW spectroscopy
  - ✓ 5 - 42 GHz
  - ✓ 6 Hz pulsed nozzle to inject the supersonic molecular beam (~ Mach 2)
- ✓ $T_{rot}$ ~ 1-3 K
- ✓ DC discharge of a mixture of Ammonia and Silane, heavily diluted in a Ne buffer

# *Experimental setup - MW-MW DR*

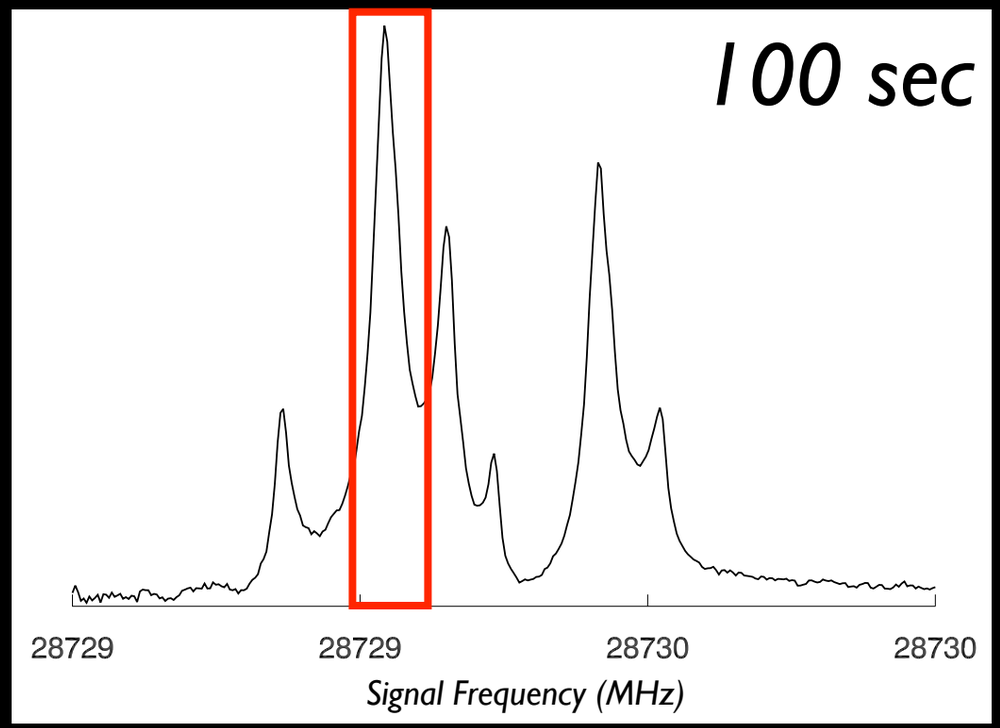
- ✓ Only the fundamental rotational transition in our FTMW spectrometer range
- ✓ MW - MW Double Resonance technique used to extend the observable range up to 60 GHz
- ✓ A second synthesizer coupled into a frequency quadrupler



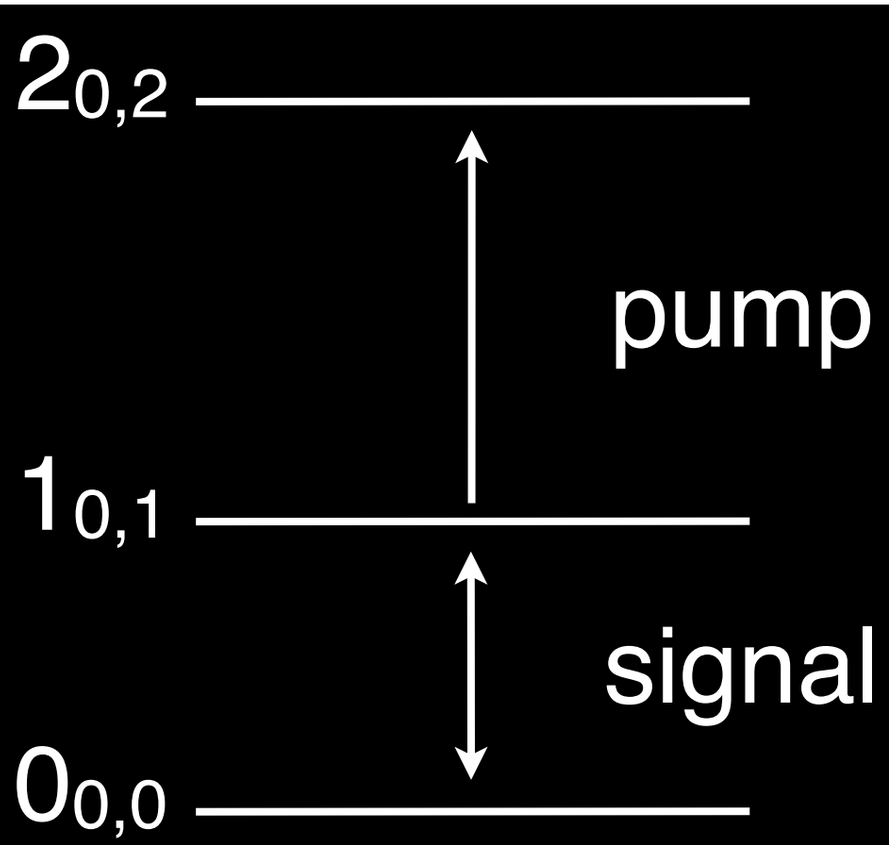
# FTM data

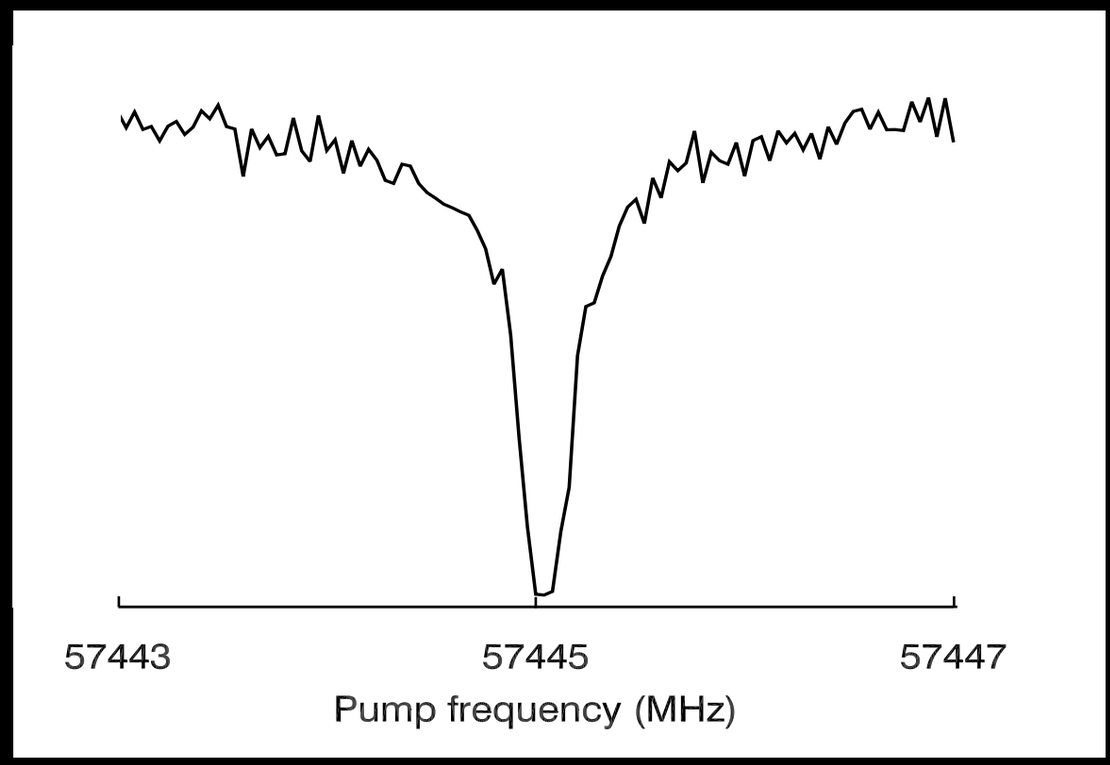


# *MW-MW double resonance*



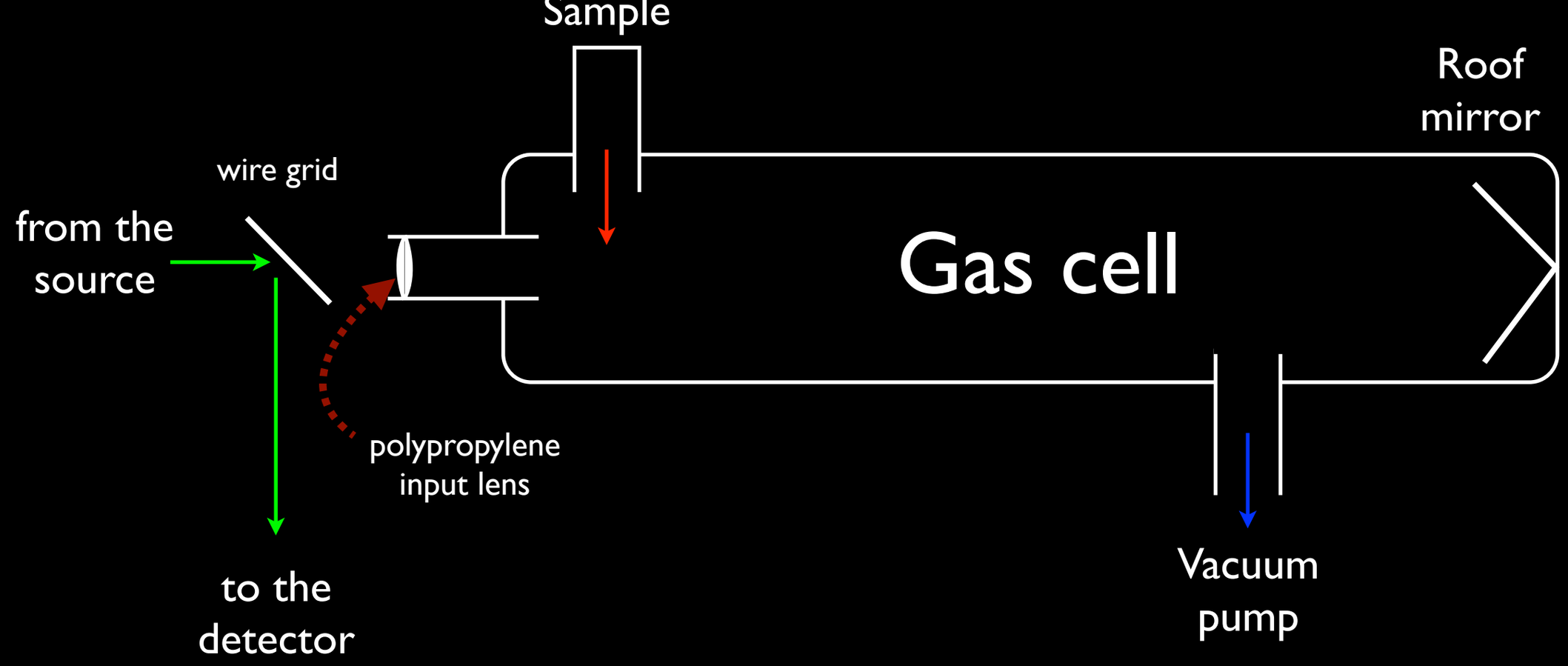

- ✓ 40 kHz/step
- ✓ 1.5 s/step
- ✓ 3 scans average



# *Experimental setup - mm-wave*

- ✓ Mixture of $SiH_4$ and $N_2$ in a -125 °C vacuum cell
- ✓ 4 $K_a$ = 0 lines detected with our mm-wave absorption spectrometer in the 256-341 GHz range



# *Isotopic confirmation*

- ✓ Theoretical rotational constants derived through structure calculation
- ✓ Scaling predicts frequencies better than 0.1%
- ✓ In same case $SiD_4$ replaced regular silane
- ✓ Fundamental rotational transition detected for 8 isotopic species:
  - ✓ *$H^{29}SiNH_2$ , $H^{30}SiNH_2$ , $HSiND_2$ , $D^{30}SiNH_2$ , $DSiND_2$ , $D^{30}SiND_2$* , and *$H^{30}SiND_2$*
- ✓ These observations provided the key confirmation before DR and mm-wave experiments

# *Conclusion*

- ✓ So far, 6 $K_a = 0$ lines detected in our lab
- ✓ Accordance up to 0.05 % of the rotational constants to the calculated value
- ✓ More mm-wave measurements to come to extend the present dataset
- ✓ Search for the other isomer *$HNSiH_2$*

# *Acknowledgments*

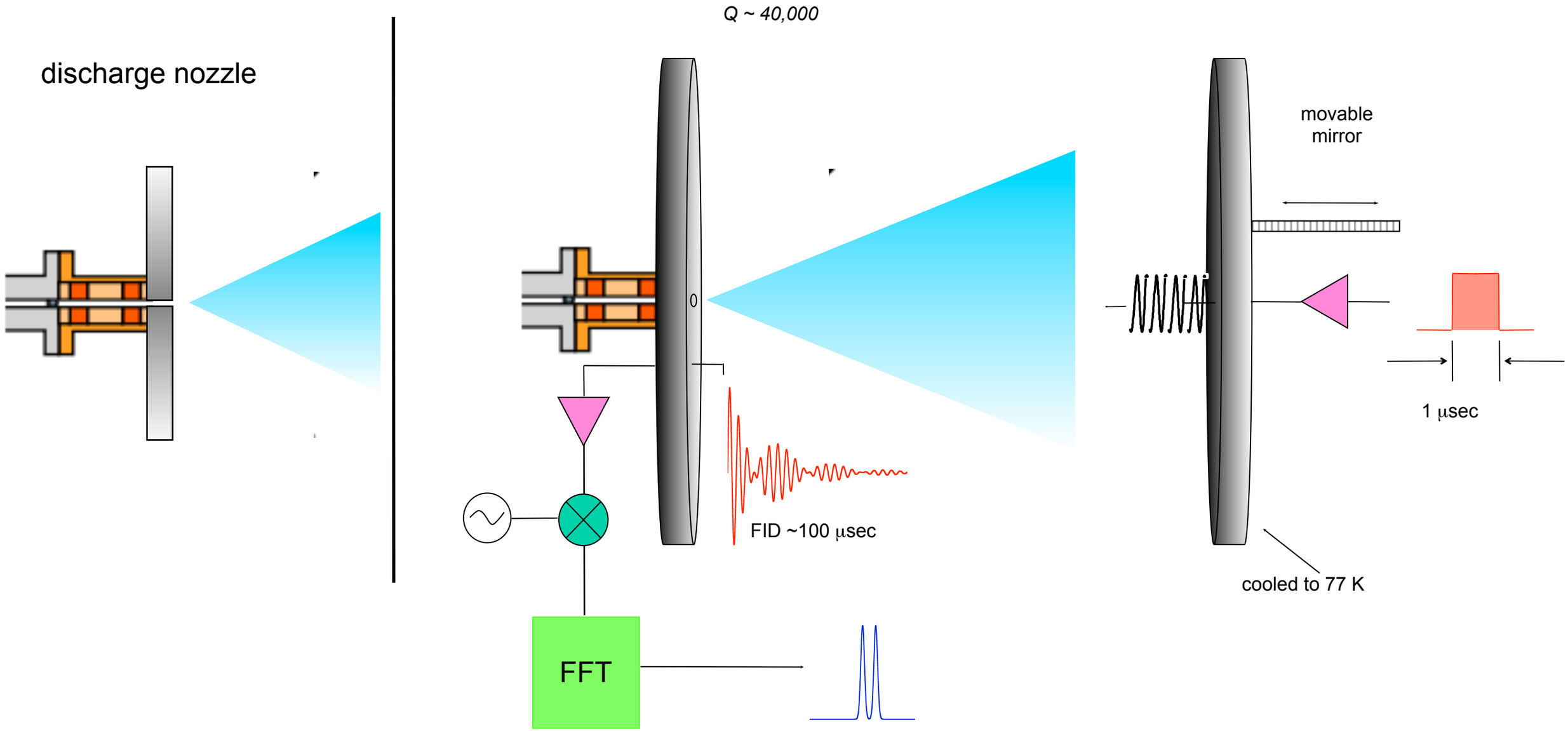

✓ Harvard-Smithsonian Center for Astrophysics

✓ NSF - NASA

✓ Damian Kokkin

✓ Brooks Pate

# FTM spectrometer




*credit M. C. McCarthy*

# *Analysis*

✓ 3 lowest $K_a = 0$ lines measured

| $J'_{K'a,K'c} \leftarrow J_{Ka,Kc}$ | Freq (MHz) | O - C (kHz) |
|---|---|---|
| $1_{0,1} \leftarrow 0_{0,0}$ | 13684.273 | 6 |
| $2_{0,2} \leftarrow 1_{0,1}$ | 27366.870 | -5 |
| $3_{0,3} \leftarrow 2_{0,2}$ | 41046.170 | 1 |

✓ 2 rotational constants fitted to ~ 0.5 %

| Const (MHz) | Exp. | Theor. |
|---|---|---|
| *A* | 101157.025 | 101157.025 |
| *B* | 7064.298(206) | 7105.729 |
| *C* | 6619.983(203) | 6631.755 |